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Major Conformations of the Ligand Skeleton of a Tetranuclear Dysprosium(III) Tartrate Complex

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Abstract

The major conformations of the ligand skeleton of the tetranuclear dysprosium(III) complex - bis(d-tartrato)bis(l-tartrato)tetradysprosate ion Dy4(d-L)2 (l-L)4- 2 (I) (d-H4L stands for d-tartaric acid, l-H4L stands for l-tartaric acid) - were found by the molecular mechanics method (the MIND program, the Dashevskii-Plyamovatyi-Kabachnik model). The calculated theoretical constants mPt for the so-called "compact" conformations of I with the tartrato ligands in the gauche conformation are consistent with the experimental paramagnetic birefringence constants (mPe) of complex I.